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OECD Benchmark for Uncertainty Analysis in Best-Estimate Modelling (UAM) for Design, Operation and Safety Analysis of LWRs - Fifth Workshop (UAM-5)

UPM Results
BWR-PWR Exercise I-1
by MCNP5 code

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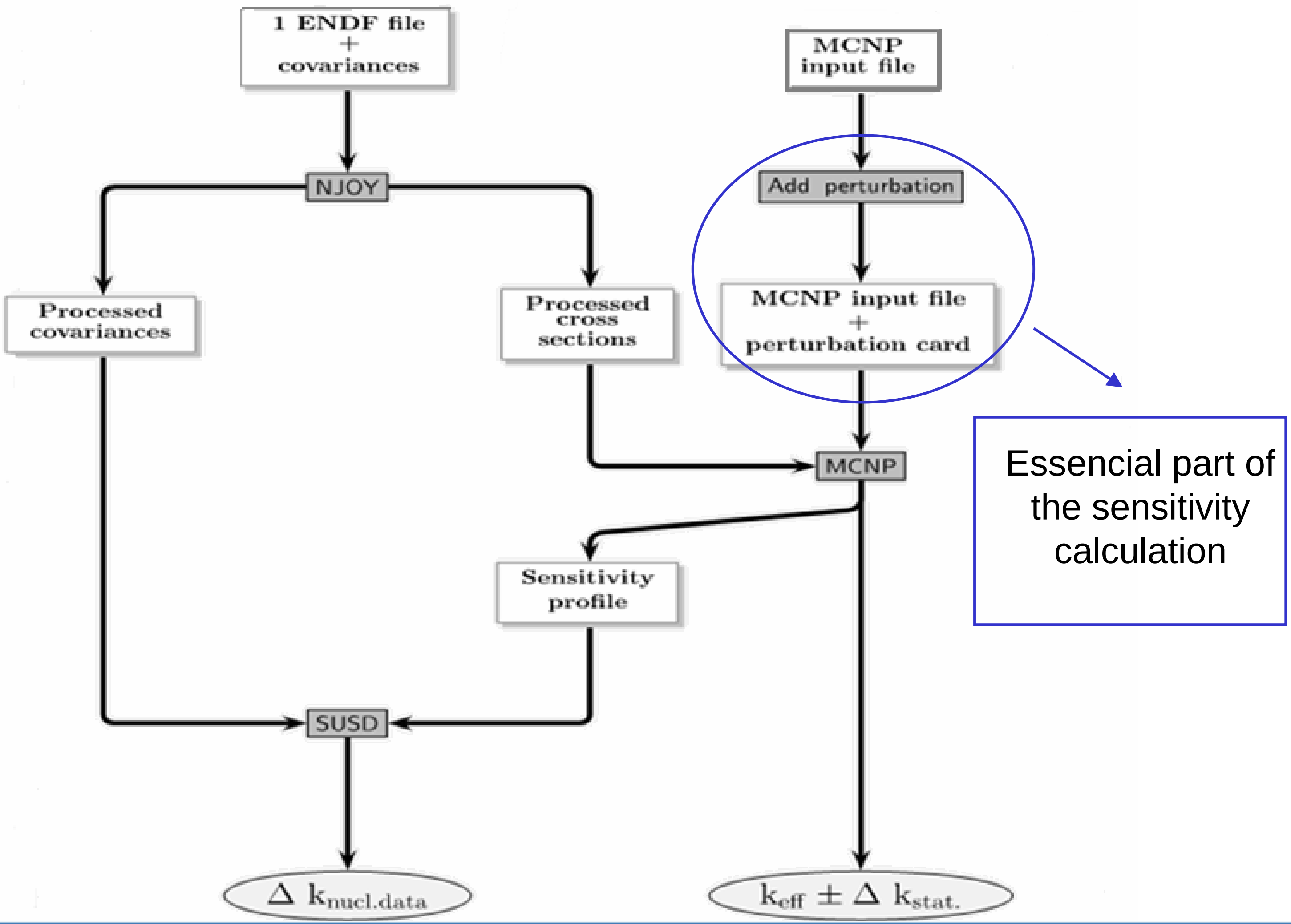
Perturbation approach

The perturbation approach relies in principle on a unique "**NJOY + MCNP5 + SUSD3D**" calculation. The inputs are the geometry MCNP5 input file and an ENDF file containing covariances.

- ENDF file, ENDF/B-VII, is processed by NJOY at different temperatures in ACE format. Ref: ***T. Viitanen and J. Leppänen,, NEA-1854 ZZ-SERPENT117 - ACELIB***
- ENDF Covariances can be processed with NJOY (used by SUSD3D).
- ANGELO, LAMDA and NJOY codes are used to generate processed covariances in 44g to SUSD3D code
- Sensitivity profiles (elastic, inelastic, capture, fission and 2,2n) are processed to SUSD3 code



Ref. "Nuclear data uncertainty propagation: Perturbation vs. Monte Carlo", D. Rochman, A. J. Koning, S. C. van der Marck, A. Hogenbirk, C. M. Sciolla, Annals of Nuclear Energy 38 (2011) 942–952

Using MCNP to Compute Sensitivities

A Taylor series expansion of a response k with respect to some reaction XS is given by:

$$k(\sigma_x) = k_0 + \left.\frac{dk}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x + \frac{1}{2}\left.\frac{d^2k}{d\sigma^2_x}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2 + \ldots$$

The MCNP5 perturbation method uses only two Taylor terms and no-cross term:

$$\left[\Delta k(\Delta\sigma_x)\right]_{PERT} = \left[\Delta k(\Delta\sigma_x)\right]_{1^o} + \left[\Delta k(\Delta\sigma_x)\right]_{2^o}$$

where: $\left[\Delta k(\Delta\sigma_x)\right]_{1^o} = \left.\frac{dk}{d\sigma_x}\right|_{\sigma_{x,0}}$ and: $\left[\Delta k(\Delta\sigma_x)\right]_{2^o} = \frac{1}{2}\left.\frac{d^2k}{d\sigma^2_x}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2$

The relative perturbation of the cross section is: $p_x \equiv \frac{\Delta\sigma_x}{\sigma_{x,0}}$

And, the sensitivity of k with respect to the cross section is: $S_{k,\sigma x} = \frac{1}{k_0 p_x}\left[\Delta k(\Delta\sigma_x)\right]_{1^o}$

Ref., “Eigenvalue sensitivity analysis using the MCNP5 perturbation capability. Favorite, J.A., In: Proc. Meeting ANS Nuclear Criticality Safety, Division, NCSD-2009, September 13–17, Richland, Washington USA.

MCNP5 PERT card

To compute sensitivities coefficients we used the **PERT card** of MCNP5.

The PERT-card is created specifying that the relevant material is replaced by the perturbated material in each of the cells in wich the material is present.

Perturbation cards are given for all energy groups (44). At the end we have **880 PERT-cards:** (4 isotopes X 5reactions X 44 groups).

Specifies the perturbeted density of the cell.

Specifies the perturbacion material number.

Indicates wich cells are parturbated.

```
PERT1:N   CELL=10  MAT=11                              RHO=7.02054E-02
          RXN= 2   ERG=8.1873E+00,2.0000E+01  METHOD=2
……………………………………
……………………………………
```

Entries must be ENDF/B reaction types that identify one or more specific reactions cross section s to perturb.

The two entries specify an energy range in wich the perturbacion is applied.

Specifies the number of terms to include in the perturbation.
In our case we include only first order (2).

PERT card's limitations

- There is no limit to the number of perturbations, but they should be kept to a minimum.

- Large perturbations require higher than second order terms to avoid inaccurate tallies.

- The track length estimate of keff in KCODE critically calculations assumes the fundamental eigenvector (fission distribution) is unchanged in the perturbated configuration.

  So, the accuracy is limited because the "*differential operator method*" does not account for this perturbation.

- Scattering affects the fission source spatial distribution more than capture does – so the error in: S_{k,σ_s} , can be large.

- It doesn't allow to calculate chi and nu-bar.

Ref., "Eigenvalue sensitivity analysis using the MCNP5 perturbation capability. Favorite, J.A., In: Proc. Meeting ANS Nuclear Criticality Safety, Division, NCSD-2009, September 13–17, Richland, Washington USA.

SUSD3D: $(\Delta k_{eff})^2 = (T)\cdot[V]\cdot(T)^T$

Figure 4. SUSD3D input

```
PWR-HZP UAM, Exerc I.1

unit   20  21  22  22

mode   1 1 1 0 /

ovly   3 /
grp  44  0
end
c*
c* data for overlay-3
mat  825 0   0 /
mt  2 4 16 18 102 /
mat  9225 0   0 /
mt  2 4 16 18 102 /
mat  9228 0   0 /
mt  2 4 16 18 102  /
mat  9237 0   0 /
mt  2 4 16 18 102 /
end
c*
c* end of run
stop
```

20→ GENDF cross section input file unit
21→ sensitivity coefficients output file unit
22→ covariance matrix input file unit
22→ sed/sad covariance input file unit

0→ non-multiplying medium
1→ fission cross section is in MT18

We used the OVERLAY3 card that calculates the variance and the relative standard deviation of the response from the sensitivity coefficients and the covariance matrices.

Mat→ number of the nuclide to be analysed: O-16, U-234, U-235 and U-238
MT→ definition of reaction types: 2 → elastic
4 → inelastic
16 → (n,2n)
18 → fission
102 → capture

Reaction rates prediction

Table 1. Definition of power density for pin cells problems

		BWR	PWR
Nominal power	P_0 (MWt)	3293	2772
Relative power	P/P_0	1	1
Active height	H_0 (cm)	365.03	357.12
Linear fuel density	r_A(gU/cm)	10.5895	6.2784
Number F/Assemblies	$N_{F/A}$	764	177
Number of rods per F/A	N_r	49	208
Power density	W/gU	22.76	33.58

$$\text{power density} = \frac{((P/P_0)\cdot P_0)}{\left(H_0 \cdot N_{\mathrm{F/A}} \cdot N_r \cdot rA\right)}$$

$$flux_{total} = flux_{MCNP5} \cdot FMF$$

$$FMF = \frac{(Power_{rod} \cdot \nu)}{(1.602E-13 \cdot Q_{fis} \cdot k_{eff})}$$

$$Q_{fis} = 1.29927 \cdot 10^{-3}(\mathrm{Z}^2 \mathrm{A}^{0.5}) + 33.12$$

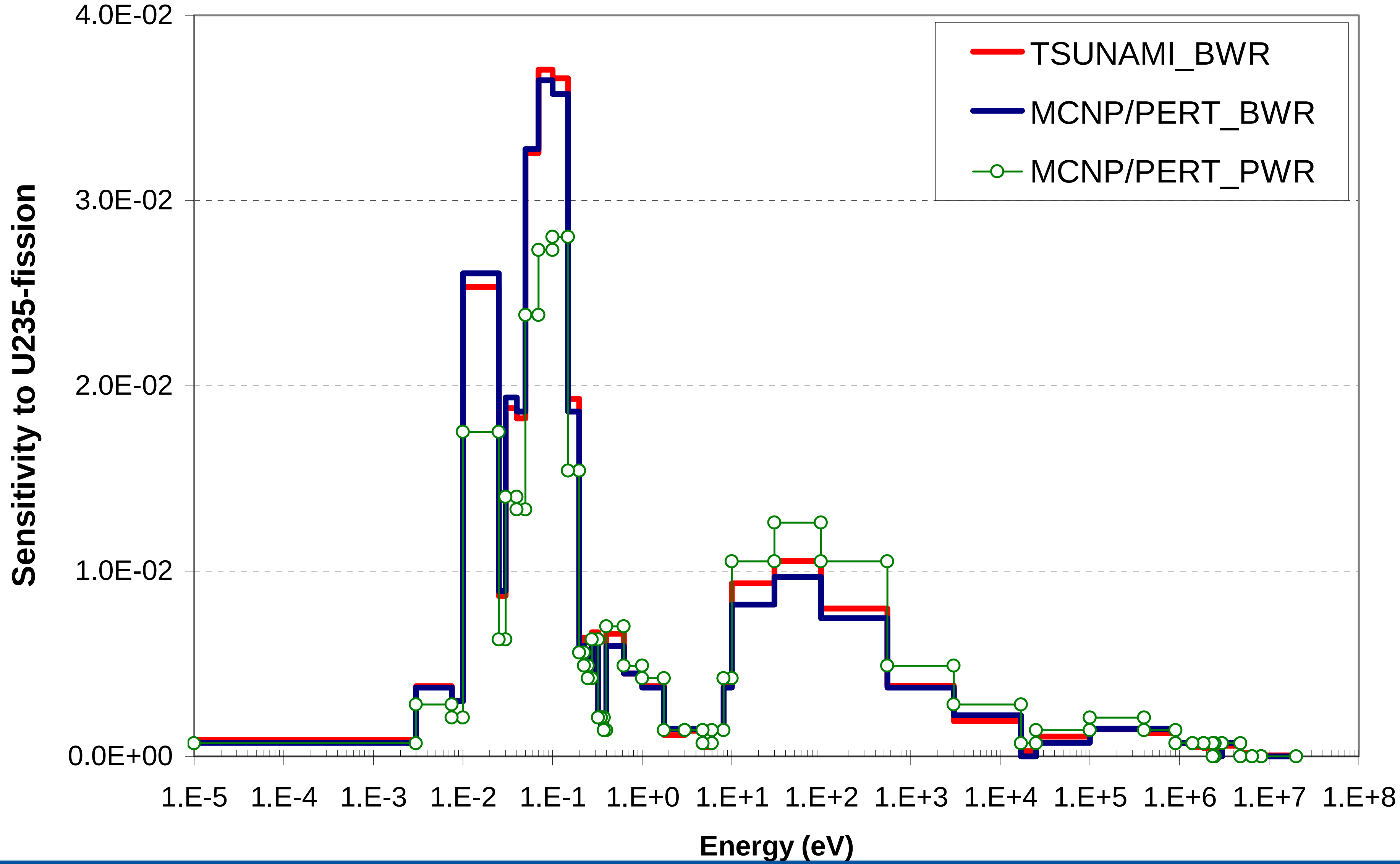
Ref. A.G. Croff. Origen2: A versatile computer code for calculating the nuclide compositions and characteristics of nuclear materials. *Nucl. Technol.*, 62(3), 1983.

MCNP5 uses a Q-value that only takes into account the kinetic energy of prompt particles and not for the delayed ones.
We have to use neutron fluence instead of heating energy calculated by MCNP5 and use a correct Q-value.

$$\text{reaction rate} = N \cdot flux_{total} \cdot \sigma_{eff}$$

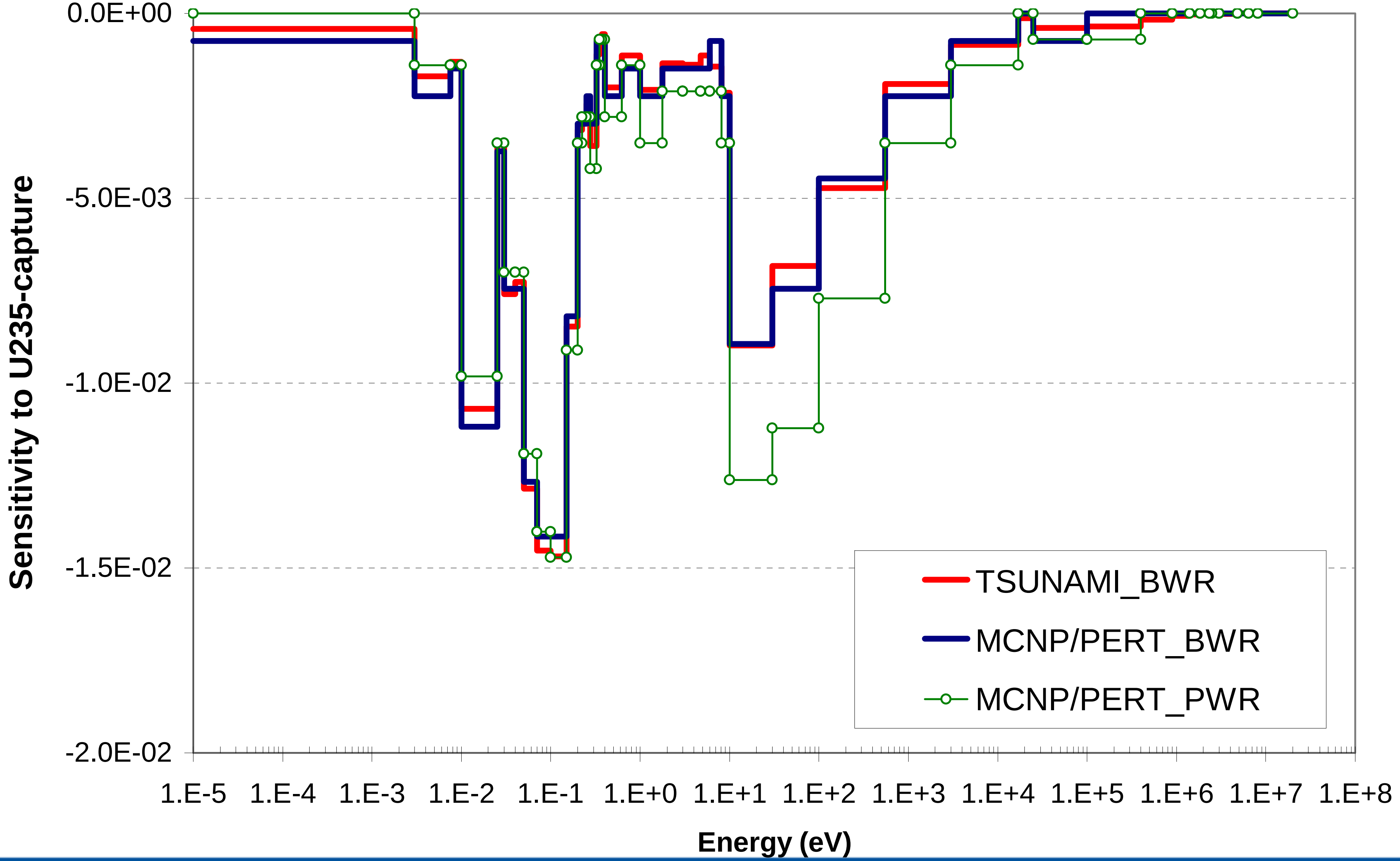
Sensitivity Coefficients (HZP)

- U235-fission: Good agreement TSUNAMI - MCNP/PERT



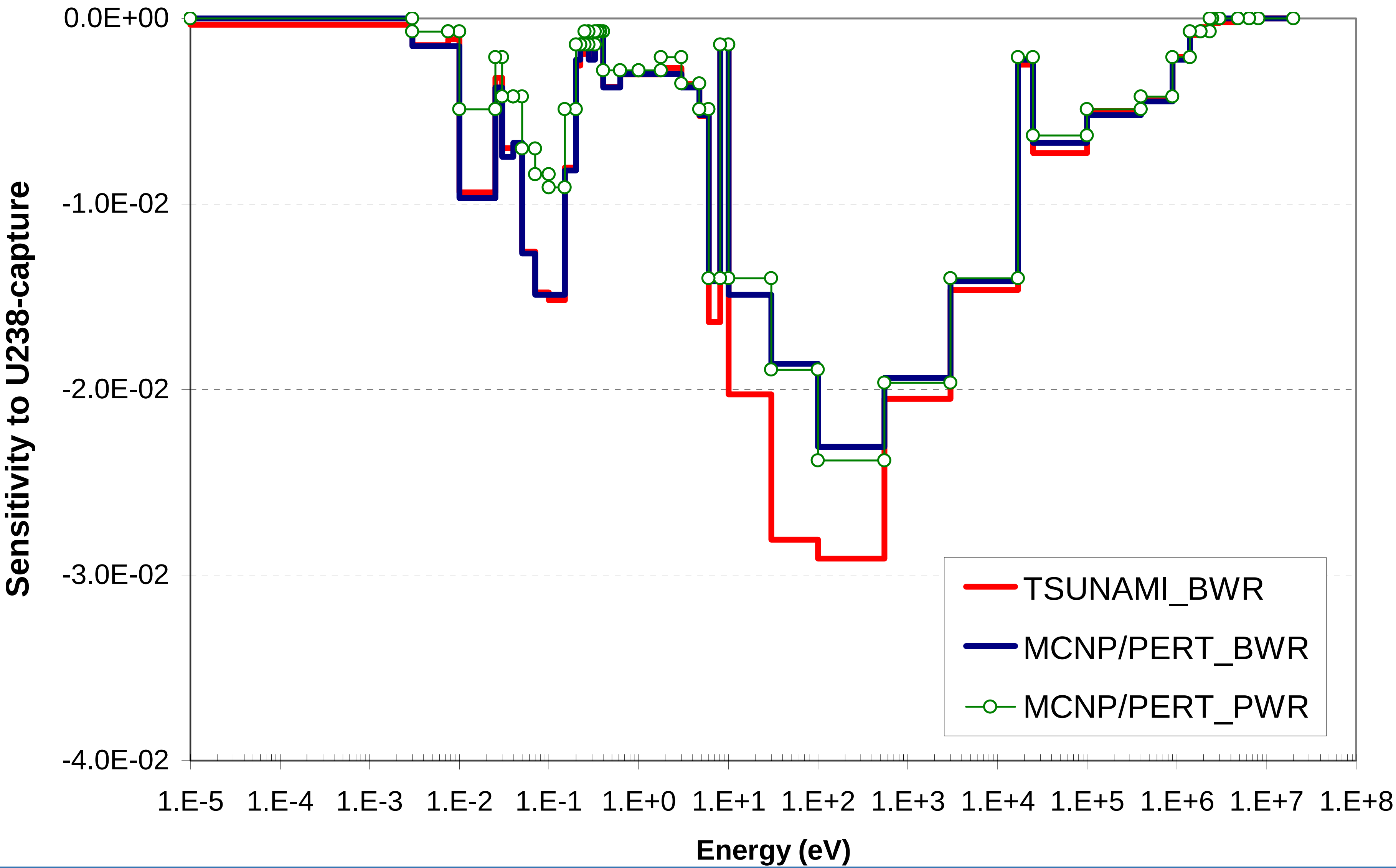
Sensitivity Coefficients (HZP/PWR)

- U235-capture: Good agreement TSUNAMI - MCNP/PERT



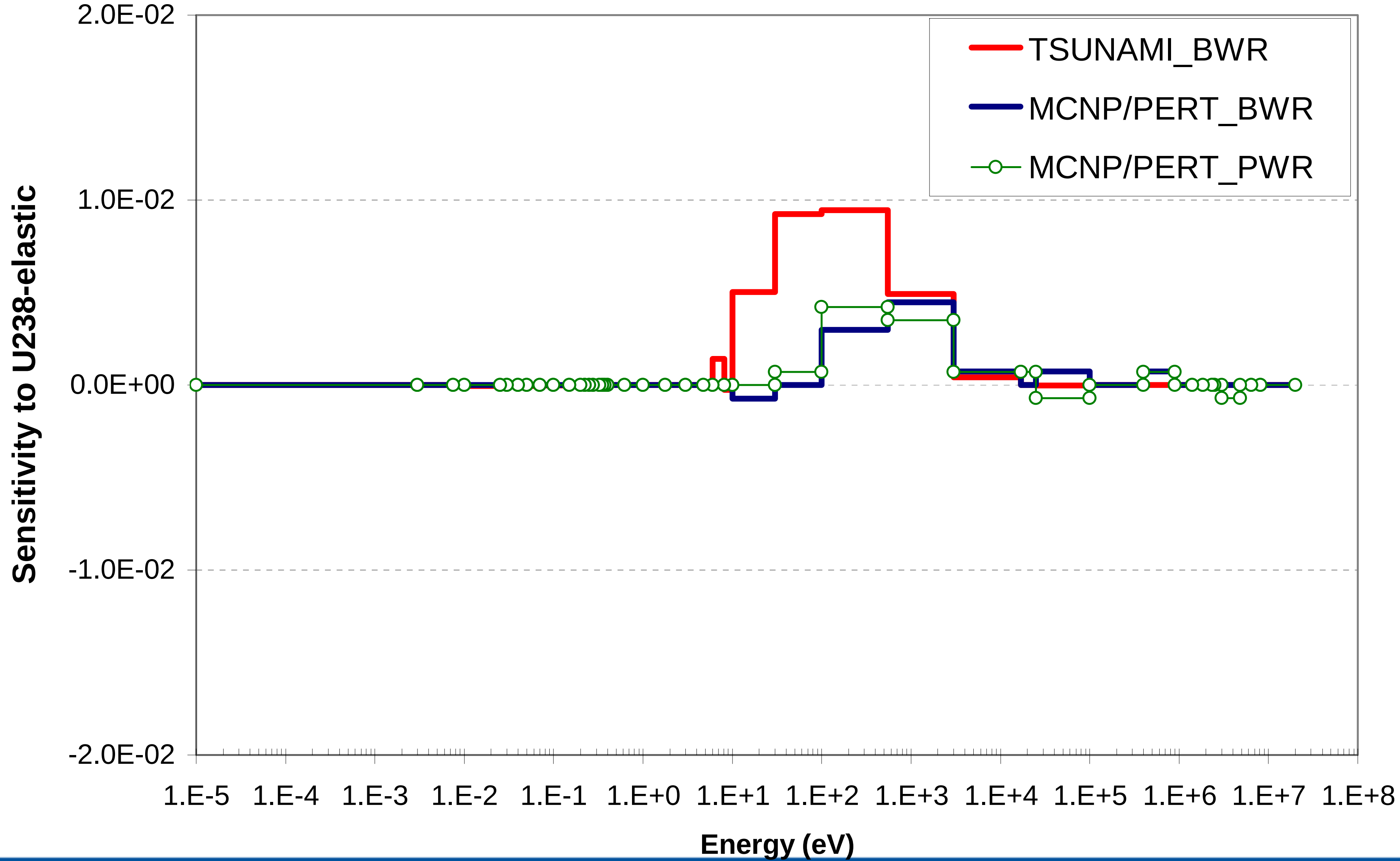
Sensitivity Coefficients (HZP/PWR)

- U238-capture: Differences between 10eV-10^3 eV

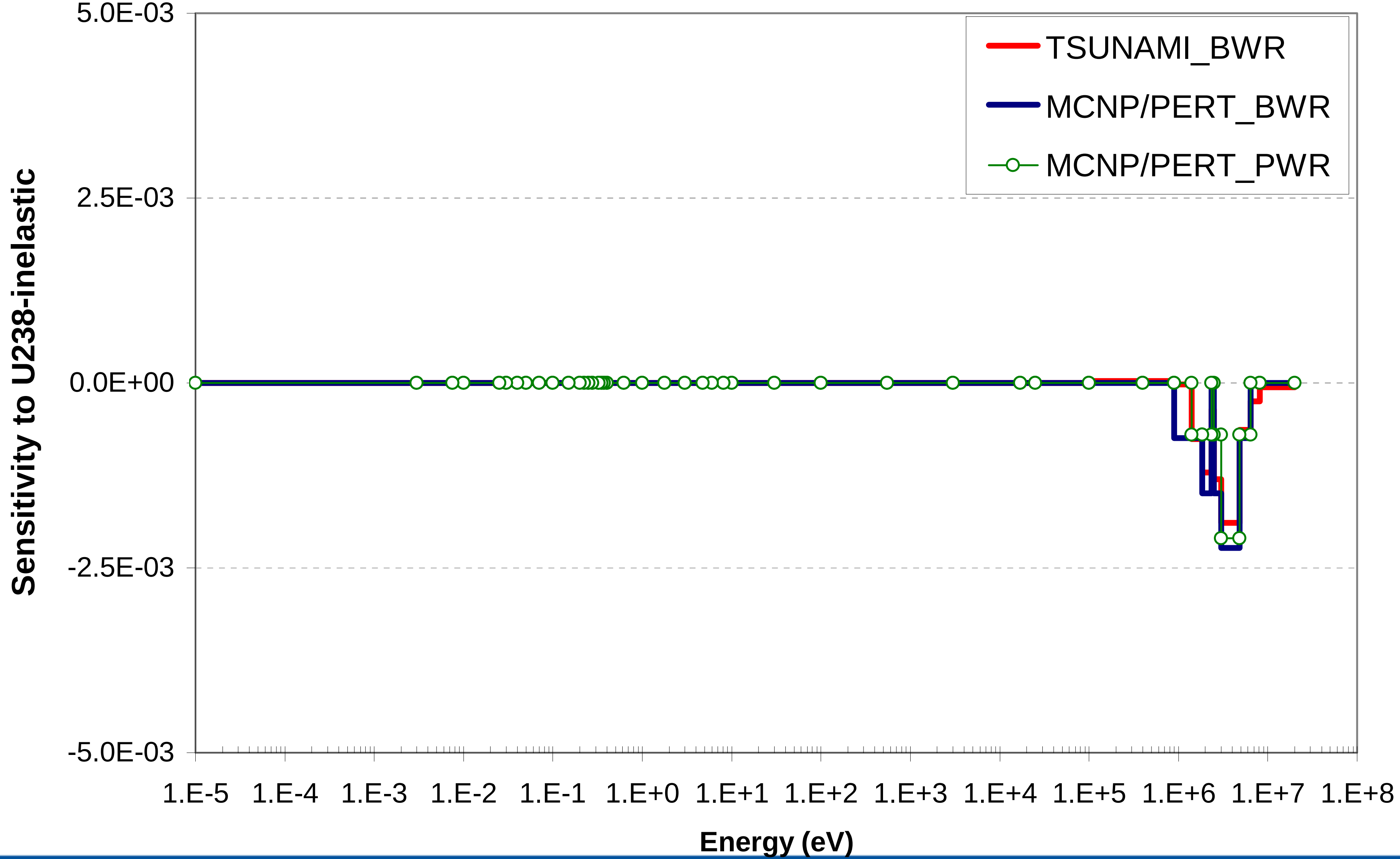


Sensitivity Coefficients (HZP/PWR)

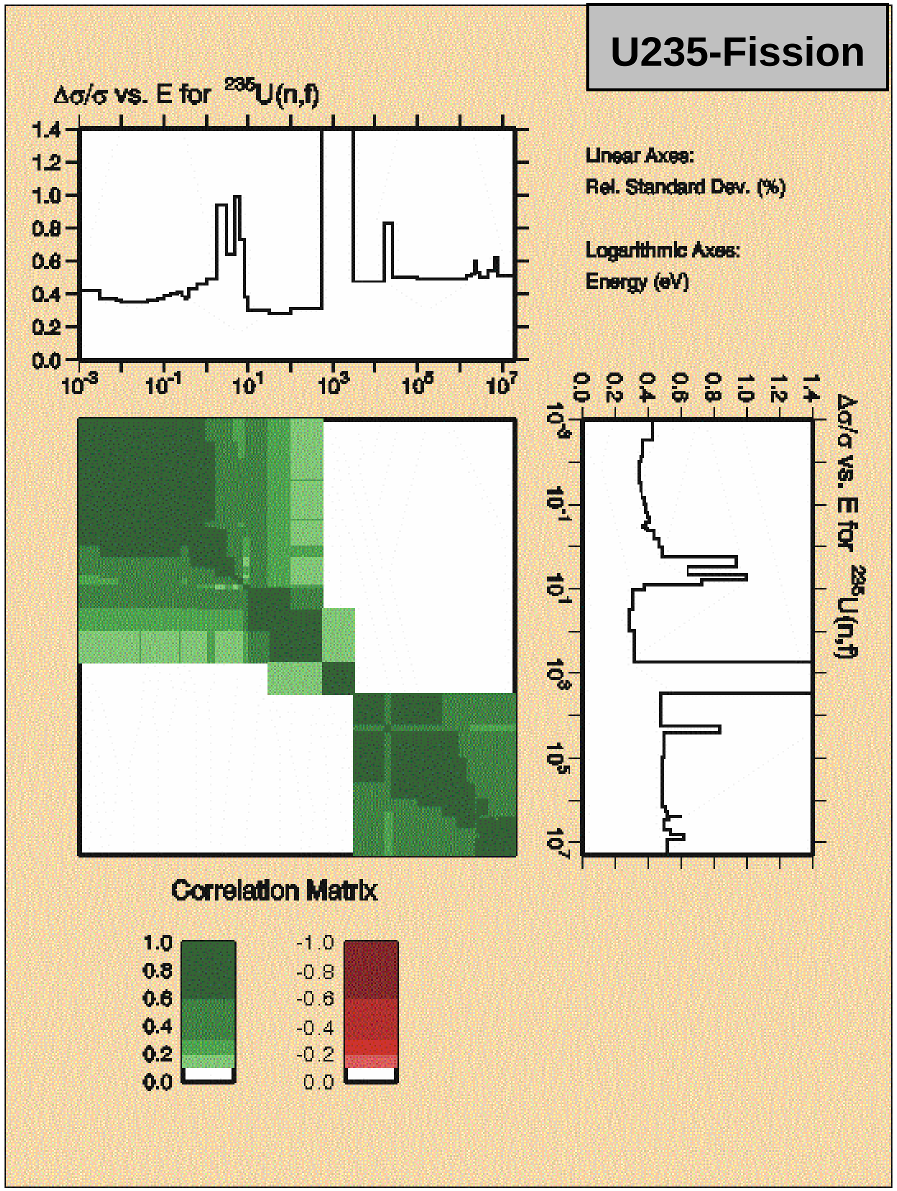
- U238-capture: Differences between 10eV-10^3 eV

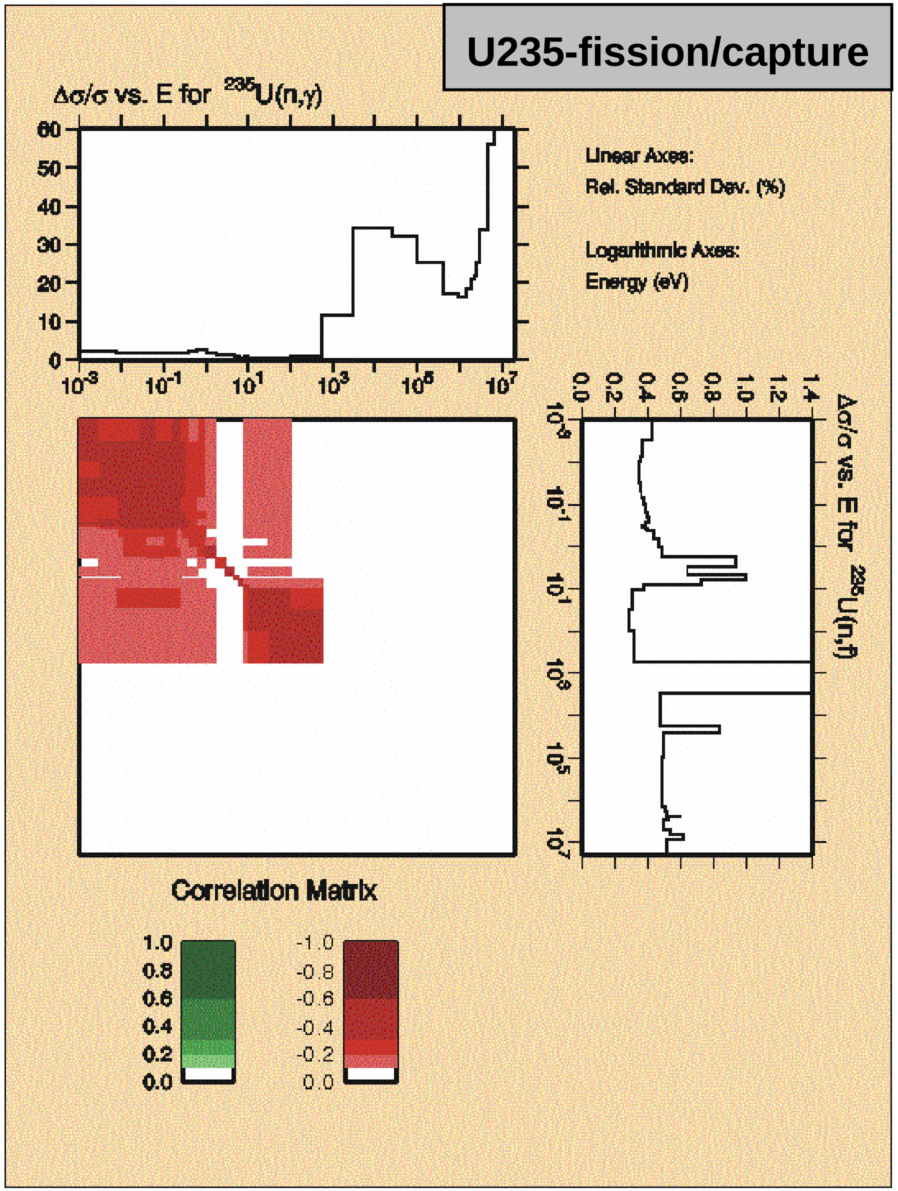


Sensitivity Coefficients (HZP/PWR)

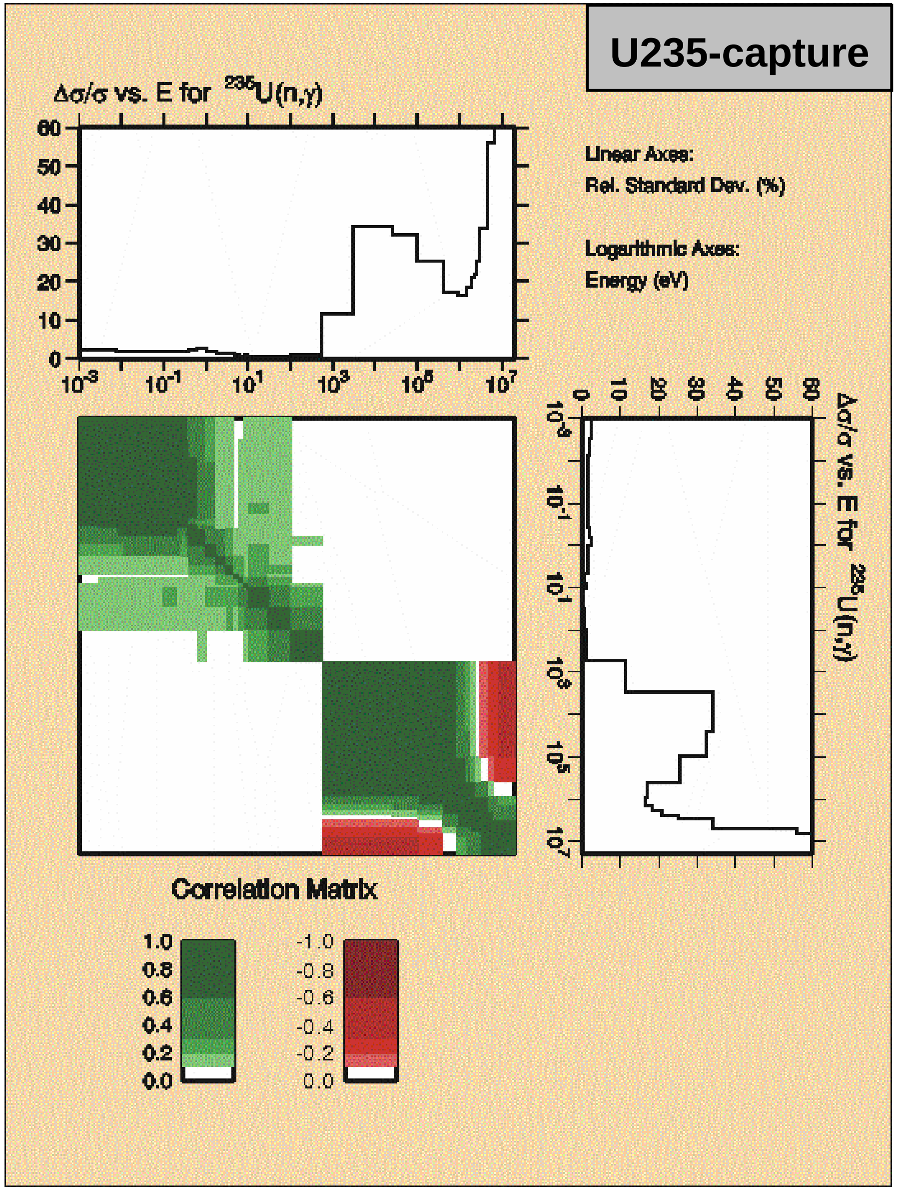


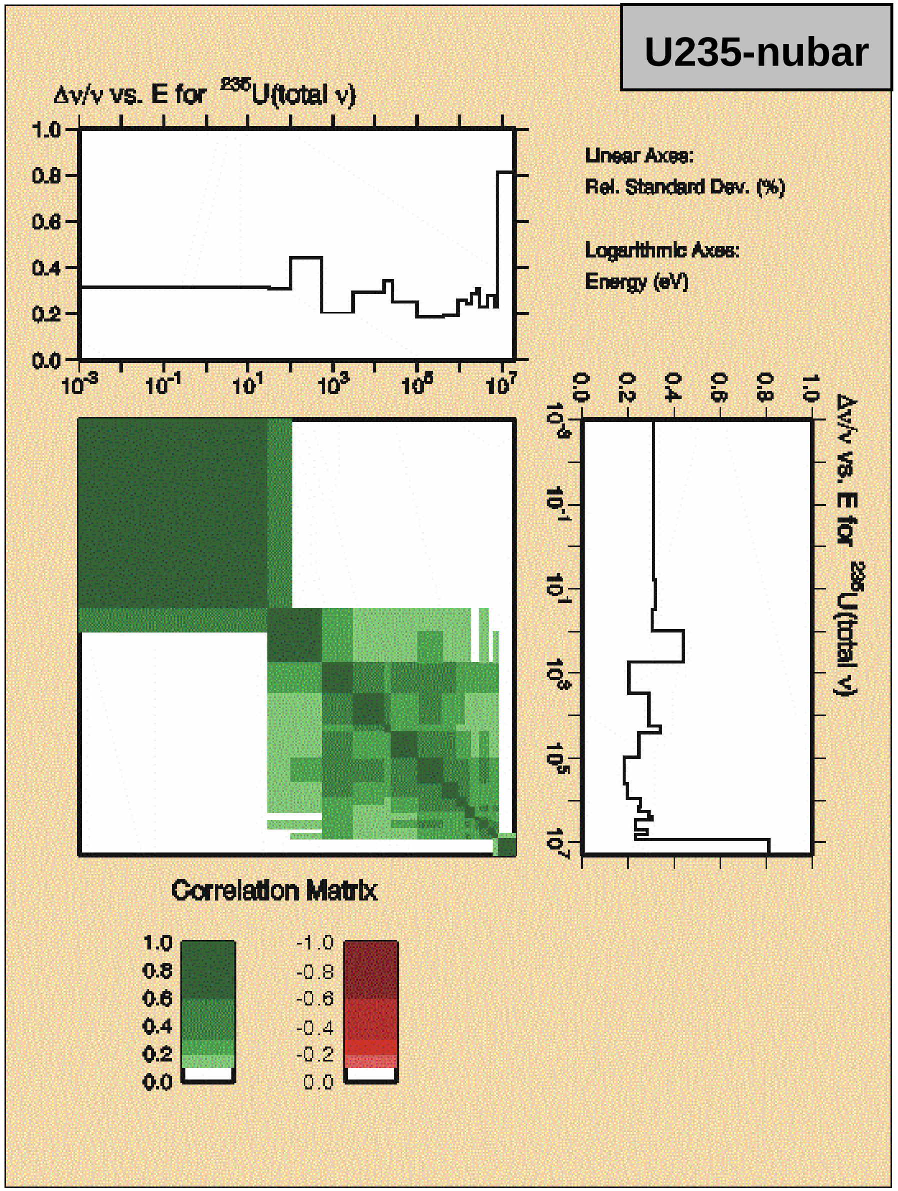
SCALE6.0 Uncertainties





SCALE6.0 Uncertainties





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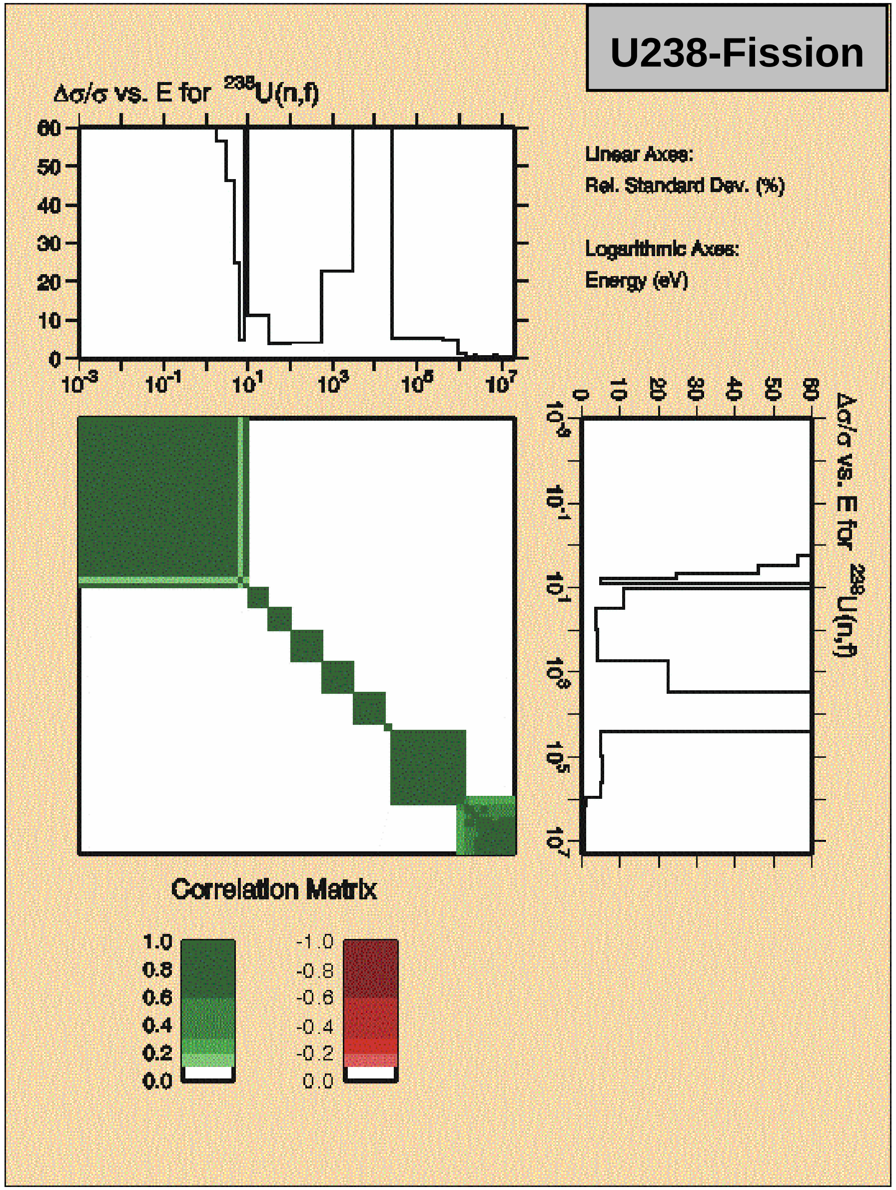
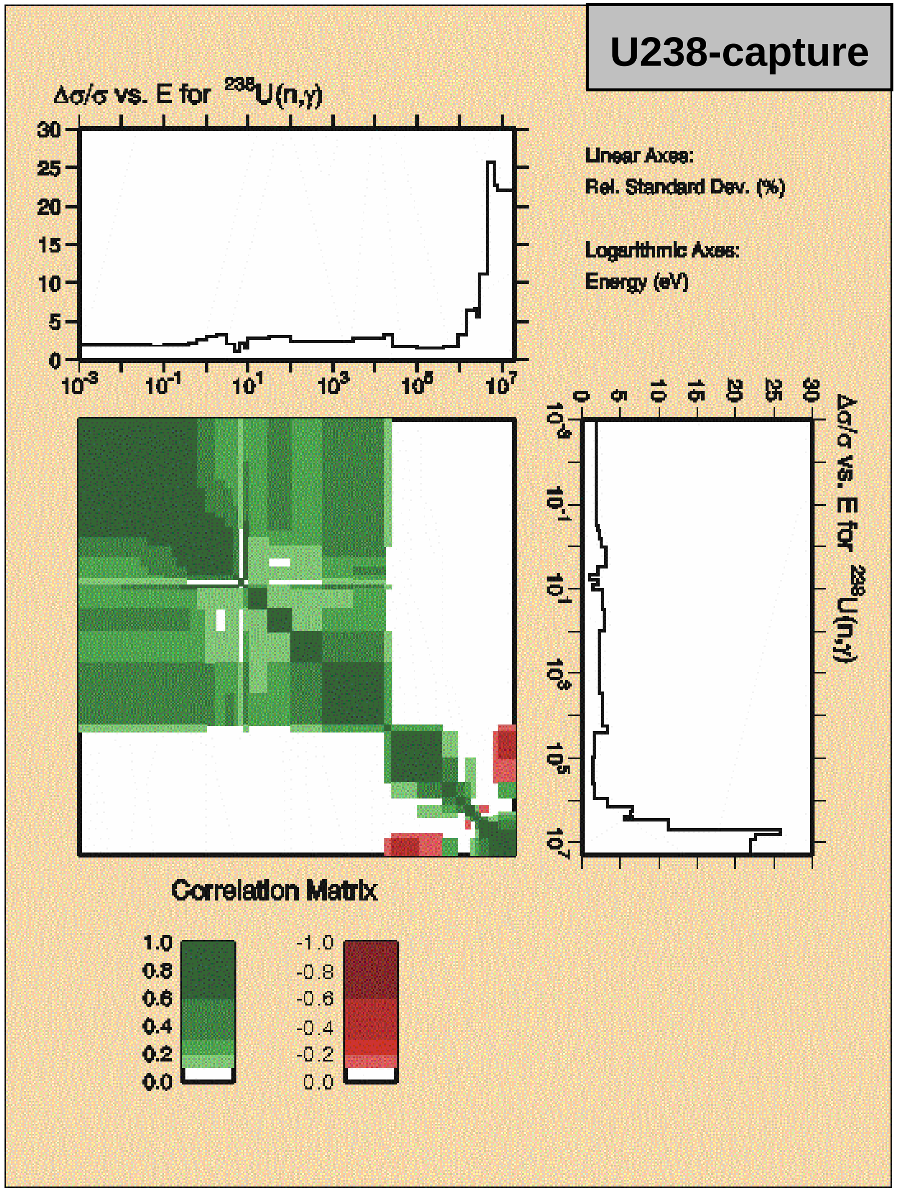
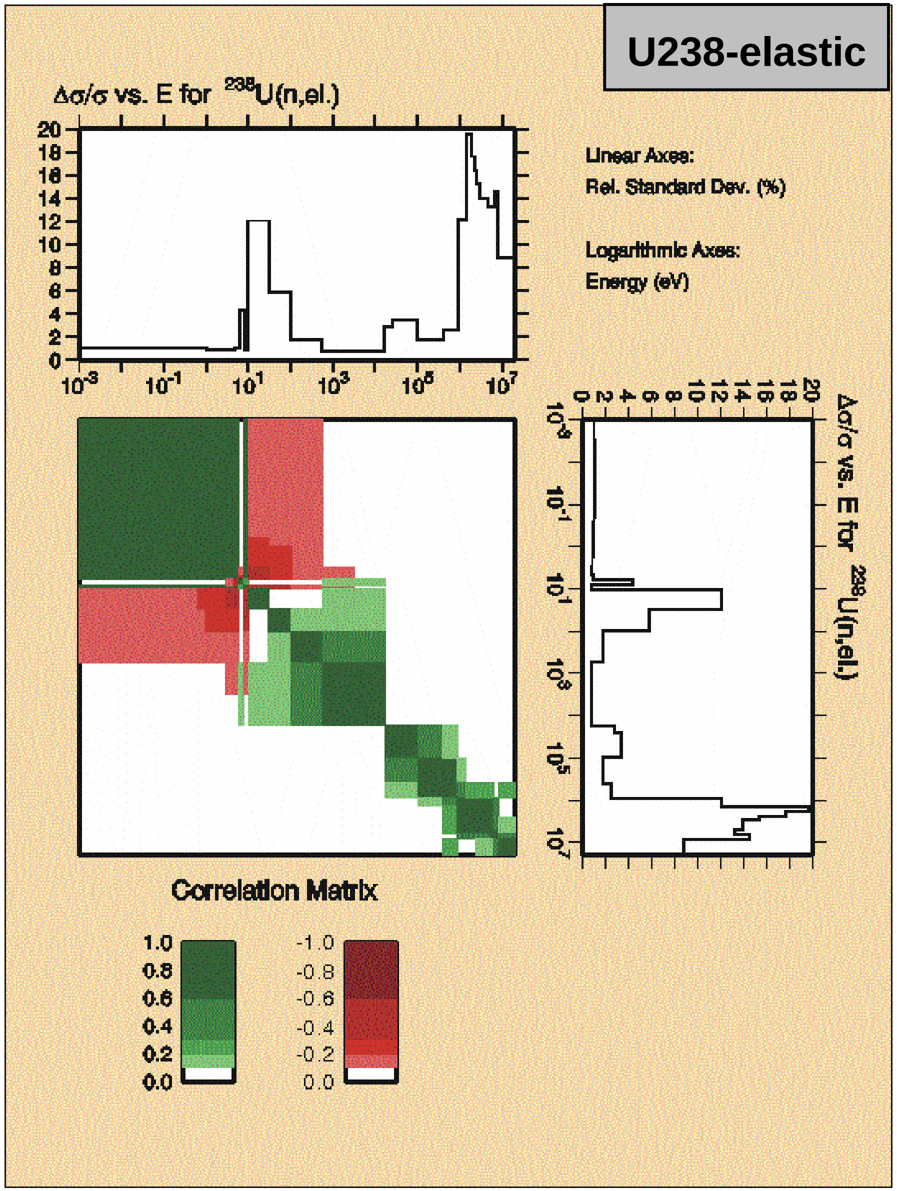
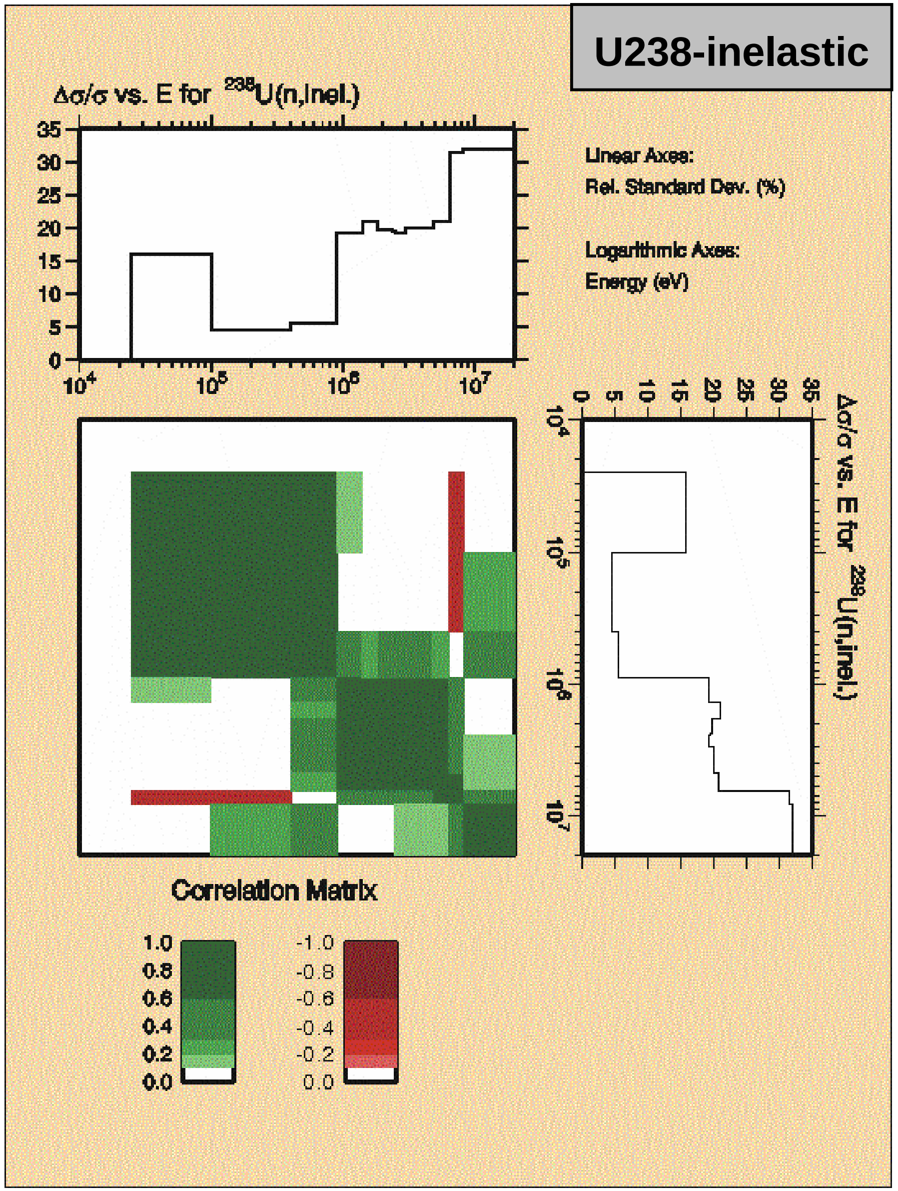
SCALE6.0 Uncertainties





SCALE6.0 Uncertainties





RESULTS: BWR

		Hot Zero Power -BWR		Hot Full Power -BWR	
		MCNP	KENO	MCNP	KENO
	Kinf	1.34233+-0.00033	1.33340+-0.0026	1.33036E+00 +- 0.00032	1.32060+-0.00250
	Uncertanties (%Δk/k)	0.4182	0.5444	0.41439	0.5551
	U238-capt	0.3151	0.3464	0.3199	0.3551
	U235-capt	0.1810	0.1831	0.1817	0.1829
Top contributors	U235-fiss	0.0939	0.0949	0.0940	0.0948
the uncertainty	U238-n,n'	0.1415	0.1226	0.1156	0.1328
	U235-fiss-capt	0.1599	0.1136	0.1601	0.1134
	U235-nubar	-	0.2713	-	0.2706
Absortion rate ($cm^{-3}s^{-1}$)	U235	2.8566E+09	2.89E+09	2.85238E+12	2.90E+12
	U238	7.1705E+09	7.22E+09	7.94771E+12	7.54E+12
Uncertainties	U235	0.3906	-	0.3973	-
	U238	0.5210	-	0.5347	-
Fission rate ($cm^{-3}s^{-1}$)	U235	1.3195E+10	1.32E+10	1.31688E+13	1.32E+13
	U238	7.9943E+08	8.02E+08	8.12176E+11	8.21E+11
Uncertainties	U235	0.4316	-	0.4380	-
	U238	3.7312	-	3.7526	-

RESULTS: PWR

		Hot Zero Power -PWR		Hot Full Power -PWR	
		MCNP	KENO	MCNP	KENO
	Kinf	1.42701E+00 +- 0.00034	1.42190+-0.00310	1.41130E+00 +- 0.00036	1.40510+-0.00290
	Uncertanties (%Δk/k)	0.36719	0.5029	0.37336	0.5125
	U238-capt	0.2535	0.2877	0.2607	0.2977
	U235-capt	0.2095	0.2124	0.2109	0.2128
Top contributors	U235-fiss	0.0770	0.0776	0.0769	0.0777
the uncertainty	U238-n,n'	0.0944	0.1058	0.0954	0.1096
	U235-fiss-capt	0.1470	0.1050	0.1472	0.1049
	U235-nubar	-	0.2646	-	0.2633
Absortion rate ($cm^{-3}s^{-1}$)	U235	2.09330E+09	2.11E+09	2.10302E+12	2.13E+12
	U238	3.99122E+09	4.04E+09	4.1816E+12	4.24E+12
Uncertainties	U235	0.3632	-	0.3699	-
	U238	0.5431	-	0.5621	-
Fission rate ($cm^{-3}s^{-1}$)	U235	8.92751E+09	8.92E+09	8.91203E+12	8.91E+12
	U238	4.88051E+08	4.91E+08	4.99342E+11	5.04E+11
Uncertainties	U235	0.3991	-	0.4078	-
	U238	3.5985	-	3.6499	-

Note: We have identified a problem processing SCALE6.0/COVA libraries with ANGELO code. Some cross-correlations are not considered, (e.g. nelasl-ninel for U235). The effect in the total Δk/k(%) is not significant. The correct value for HZP/PWR is Δk/k(%) =**0.36909**

ANGELO bug

ANGELO code has a problem when COVERX library format is read. The code cannot read all covariance matrix between reactions inside COVERX library. This occurs when the order of presentation of each covariance do not met a characteristic that will be showed later.

Figure 1. MAT9228 proccessed with ANGELO code

```
MATD= 9228  MTS/MTS2= 1 2
   7
WARNING: Covariance MT 1 available but not considered !
MATD= 9228  MTS/MTS2= 4 2
   14
WARNING: Covariance MT 1 available but not considered !
```

Figure 2. MAT9228 processed with VIEWCVX code

```
COVERX file name: cvx.mat92235
        view mode: covariance matrices.
 control parameters
 ------------------
 number of matrices (nmtrix) ...............     16
<< no.    8 : relative covariance matrix ... nuclide:           >>
 column material (92235,  2) and row material (92235,  1)
    row         1         2         3         4         5         6
 column  --------  --------  --------  --------  --------  --------
    1    1.178E-4  9.621E-5  7.963E-5  8.209E-5  8.620E-5  9.369E-5
    2    1.067E-4  1.082E-4  8.693E-5  8.112E-5  8.649E-5  9.522E-5
<< no.    9 : relative covariance matrix ... nuclide:           >>
 column material (92235,  2) and row material (92235,  4)
  row         1         2         3         4         5         6
column  --------  --------  --------  --------  --------  --------
    1   -1.816E-2 -9.178E-3 -3.235E-3 -6.522E-4  1.797E-4  3.901E-4
    2   -6.957E-3 -9.084E-3 -6.636E-3 -1.756E-3 -8.247E-5 -7.506E-5
```

ANGELO bug

To find a simple solution to this problem, we have to guaranty that all covariance matrix between different reactions should met the next rule: *”The first MT index of the covariance matrix should be presented in line 5d before the second MT index, when line 7d is observed”*

Figure 3. Extract of the MAT9228 coverx file, original and updated.

```
5d    8016       1     4  8016       2     4  8016      16     4  8016     102
           4  8016     103    4  8016     104     4  8016     107     4  8016       4
           4  8016     105    4
7d    8016       2  8016        1        1
```

Not read

```
5d    8016       4     4  8016       2     4  8016      16     4  8016     102
           4  8016     103    4  8016     104     4  8016     107     4  8016       1
           4  8016     105    4
7d    8016       2  8016        1        1
```

Read

These changes should be also performed on the order of **6d** lines, where the cross sections values are stored in the order showed in line **5d**